

## **APPENDIX C**

### **EQUATIONS AND PARAMETER VALUES FOR CALCULATING COPC-SPECIFIC MEDIA CONCENTRATIONS**

**(38 Pages)**

## APPENDIX C

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### LIST OF VARIABLES AND PARAMETERS

$\delta_z$	=	Dimensionless viscous sublayer thickness (unitless)
$\nu_a$	=	Viscosity of air (g/cm-s)
$\nu_w$	=	Viscosity of water corresponding to water temperature (g/cm-s)
$\Delta_a$	=	Density of air (g/cm <sup>3</sup> or g/m <sup>3</sup> )
$\Delta_w$	=	Density of water corresponding to water temperature (g/cm <sup>3</sup> )
$2$	=	Temperature correction factor (unitless)
$2_{bs}$	=	Bed sediment porosity (L volume/L sediment)—unitless
$2_{sw}$	=	Soil volumetric water content (mL water/cm <sup>3</sup> soil)
$a$	=	Empirical intercept coefficient (unitless)
$A$	=	Surface area of contaminated area (m <sup>2</sup> )
$A_I$	=	Impervious watershed area receiving COPC deposition (m <sup>2</sup> )
$A_L$	=	Total watershed area receiving COPC deposition (m <sup>2</sup> )
$A_W$	=	Water body surface area (m <sup>2</sup> )
$b$	=	Empirical slope coefficient (unitless)
$BD$	=	Soil bulk density (g soil/cm <sup>3</sup> soil)
$Br$	=	Plant-soil bioconcentration factor (unitless)
$Bv$	=	COPC air-to-plant biotransfer factor (mg COPC/kg DW plant)/(mg COPC/kg air)—unitless
$C$	=	USLE cover management factor (unitless)
$C_{BS}$	=	Bed sediment concentration (or bed sediment bulk density) (g/cm <sup>3</sup> or kg/L)
$C_d$	=	Drag coefficient (unitless)
$C_{dw}$	=	Dissolved phase water concentration (mg COPC/L water)
$C_s$	=	Average soil concentration over exposure duration (mg COPC/kg soil)
$C_{sb}$	=	COPC concentration in bed sediment (mg COPC/kg sediment)
$C_{wctot}$	=	Total COPC concentration in water column (mg COPC/L water column)
$C_{wtot}$	=	Total water body COPC concentration including water column and bed sediment (g COPC/m <sup>3</sup> water body) or (mg/L)
$C_{yv}$	=	Unitized yearly average air concentration from vapor phase (μg-s/g-m <sup>3</sup> )
$C_{yww}$	=	Unitized yearly (water body or watershed) average air concentration from vapor phase (μg-s/g-m <sup>3</sup> )
$D_a$	=	Diffusivity of COPC in air (cm <sup>2</sup> /s)
$d_{bs}$	=	Depth of upper benthic sediment layer (m)
$Ds$	=	Deposition term (mg COPC/kg soil-yr)
$d_{wc}$	=	Depth of water column (m)
$D_w$	=	Diffusivity of COPC in water (cm <sup>2</sup> /s)
$Dydp$	=	Unitized yearly average dry deposition from particle phase (s/m <sup>2</sup> -yr)
$Dytwp$	=	Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m <sup>2</sup> -yr)
$Dywp$	=	Unitized yearly average wet deposition from particle phase (s/m <sup>2</sup> -yr)

$D_{ywv}$	=	Unitized yearly average wet deposition from vapor phase ( $\text{s/m}^2\text{-yr}$ )
$D_{ywwv}$	=	Unitized yearly (water body or watershed) average wet deposition from vapor phase ( $\text{s/m}^2\text{-yr}$ )
$d_z$	=	Total water body depth (m)
$ER$	=	Soil enrichment ratio (unitless)
$E_v$	=	Average annual evapotranspiration (cm/yr)
$f_{bs}$	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
$F_W$	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$f_{wc}$	=	Fraction of total water body COPC concentration in the water column (unitless)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$H$	=	Henry's Law constant ( $\text{atm}\cdot\text{m}^3/\text{mol}$ )
$I$	=	Average annual irrigation (cm/yr)
$k$	=	Von Karman's constant (unitless)
$K$	=	USLE erodibility factor (ton/acre)
$k_b$	=	Benthic burial rate constant ( $\text{yr}^{-1}$ )
$Kd_{bs}$	=	Bed sediment/sediment pore water partition coefficient ( $\text{cm}^3 \text{ water/g bottom sediment}$ or $\text{L water/kg bottom sediment}$ )
$Kd_s$	=	Soil-water partition coefficient ( $\text{cm}^3 \text{ water/g soil}$ )
$Kd_{sw}$	=	Suspended sediment-surface water partition coefficient ( $\text{L water/kg suspended sediment}$ )
$K_G$	=	Gas phase transfer coefficient (m/yr)
$K_L$	=	Liquid phase transfer coefficient (m/yr)
$kp$	=	Plant surface loss coefficient ( $\text{yr}^{-1}$ )
$ks$	=	COPC soil loss constant due to all processes ( $\text{yr}^{-1}$ )
$kse$	=	COPC loss constant due to soil erosion ( $\text{yr}^{-1}$ )
$ksg$	=	COPC loss constant due to biotic and abiotic degradation ( $\text{yr}^{-1}$ )
$ksl$	=	COPC loss constant due to leaching ( $\text{yr}^{-1}$ )
$ksr$	=	COPC loss constant due to surface runoff ( $\text{yr}^{-1}$ )
$ksv$	=	COPC loss constant due to volatilization ( $\text{yr}^{-1}$ )
$k_v$	=	Water column volatilization rate constant ( $\text{yr}^{-1}$ )
$K_v$	=	Overall COPC transfer rate coefficient (m/yr)
$k_{wt}$	=	Overall total water body dissipation rate constant ( $\text{yr}^{-1}$ )
$L_{DEP}$	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
$L_{dif}$	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
$L_E$	=	Soil erosion load (g/yr)
$L_R$	=	Runoff load from pervious surfaces (g/yr)
$L_{RI}$	=	Runoff load from impervious surfaces (g/yr)
$L_T$	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
$LS$	=	USLE length-slope factor (unitless)

$OC_{sed}$	=	Fraction of organic carbon in bottom sediment (unitless)
$p_L$	=	Liquid phase vapor pressure of chemical (atm)
$p_s$	=	Solid phase vapor pressure of chemical (atm)
$P$	=	Average annual precipitation (cm/yr)
$PF$	=	USLE supporting practice factor (unitless)
$Pd$	=	Plant concentration due to direct deposition (mg COPC/kg DW)
$Pr$	=	Plant concentration due to root uptake (mg COPC/kg DW)
$Pv$	=	Plant concentration due to air-to-plant transfer (mg COPC/g DW plant tissue or mg COPC/kg DW plant tissue)
$Q$	=	COPC-specific emission rate (g/s)
$r$	=	Interception fraction—the fraction of material in rain intercepted by vegetation and initially retained (unitless)
$R$	=	Universal gas constant (atm-m <sup>3</sup> /mol-K)
$RO$	=	Average annual surface runoff from pervious areas (cm/yr)
$RF$	=	USLE rainfall (or erosivity) factor (yr <sup>-1</sup> )
$Rp$	=	Interception fraction of the edible portion of plant (unitless)
$SD$	=	Sediment delivery ratio (unitless)
$\Delta Sf$	=	Entropy of fusion [ $\Delta Sf/R = 6.79$ (unitless)]
$SF$	=	Slope factor (mg/kg-day) <sup>-1</sup>
$ST$	=	Whitby's average surface area of particulates (aerosols) = $3.5 \times 10^{-6}$ cm <sup>2</sup> /cm <sup>3</sup> air for background plus local sources = $1.1 \times 10^{-5}$ cm <sup>2</sup> /cm <sup>3</sup> air for urban sources
$T_a$	=	Ambient air temperature (K)
$T_1$	=	Time period at the beginning of combustion (yr)
$T_2$	=	Length of exposure duration (yr)
$T_m$	=	Melting point of chemical (K)
$Tp$	=	Length of plant exposure to deposition per harvest of edible portion of plant (yr)
$TSS$	=	Total suspended solids concentration (mg/L)
$T_{wk}$	=	Water body temperature (K)
$t_{1/2}$	=	Half-time of COPC (days)
$V_{dv}$	=	Dry deposition velocity (cm/s)
$V_{fx}$	=	Average volumetric flow rate through water body (m <sup>3</sup> /yr)
$VG$	=	Empirical correction factor
$W$	=	Average annual wind speed (m/s)
$X_e$	=	Unit soil loss (kg/m <sup>2</sup> -yr)
$Yh$	=	Dry harvest yield = $1.22 \times 10^{11}$ kg DW, calculated from the 1993 U.S. average wet weight $Yh$ of $1.35 \times 10^{11}$ kg (USDA 1994b) and a conversion factor of 0.9 (Fries 1994)
$Yh_i$	=	Harvest yield of ith crop (kg DW)

$Y_p$	=	Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m <sup>2</sup> )
$Z_s$	=	Soil mixing zone depth (cm)

### EQUATION C-1

#### SOIL CONCENTRATION DUE TO DEPOSITION (SOIL INGESTION EQUATIONS)

$$C_s = \frac{D_s \cdot [1 - \exp(-k_s \cdot tD)]}{k_s}$$

where

$$D_s = \frac{100 \cdot Q}{Z_s \cdot BD} \cdot [F_v (0.31536 \cdot V_{dv} \cdot C_{yv} + D_{yvw}) + (D_{ydp} + D_{ywp}) \cdot (1 - F_v)]$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$C_s$	Average soil concentration over exposure duration	(mg COPC/kg soil)
$D_s$	Deposition term	(mg COPC/kg soil-yr)
$tD$	Time period over which deposition occurs	100 yr
$k_s$	COPC soil loss constant due to all processes	Calculated using Equation C-2 (yr <sup>-1</sup> )
$100$	Units conversion factor	100 mg-cm <sup>2</sup> /kg-cm <sup>2</sup>
$Q$	COPC-specific emission rate	See Appendix A (g/s)
$Z_s$	Soil mixing zone depth	Untilled Soil = 1 cm
$BD$	Soil bulk density	1.5 g soil/cm <sup>3</sup> soil
$F_v$	Fraction of COPC air concentration in vapor phase	See Appendix B (unitless)

**EQUATION C-1 (Continued)**

**SOIL CONCENTRATION DUE TO DEPOSITION  
(SOIL INGESTION EQUATIONS)**

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
<i>0.31536</i>	Units conversion factor	0.31536 m-g-s/cm-:g-yr
<i>V<sub>dv</sub></i>	Dry deposition velocity	3 cm/s
<i>C<sub>yv</sub></i>	Unitized yearly average air concentration from vapor phase	(:g-s/g-m <sup>3</sup> )
<i>D<sub>ywv</sub></i>	Unitized yearly average wet deposition from vapor phase	(s/m <sup>2</sup> -yr)
<i>D<sub>ydp</sub></i>	Unitized yearly average dry deposition from particle phase	(s/m <sup>2</sup> -yr)
<i>D<sub>ywp</sub></i>	Unitized yearly average wet deposition from particle phase	(s/m <sup>2</sup> -yr)

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## EQUATION C-2

### COPC SOIL LOSS CONSTANT (SOIL INGESTION EQUATIONS)

$$k_s = k_{sg} + k_{se} + k_{sr} + k_{sl} + k_{sv}$$

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
<i>k<sub>s</sub></i>	COPC soil loss constant due to all processes	(yr <sup>-1</sup> )
<i>k<sub>sg</sub></i>	COPC loss constant due to biotic and abiotic degradation	See Appendix B (yr <sup>-1</sup> )
<i>k<sub>se</sub></i>	COPC loss constant due to soil erosion	0 yr <sup>-1</sup>
<i>k<sub>sr</sub></i>	COPC loss constant due to surface runoff	See Equation C-4 (yr <sup>-1</sup> )
<i>k<sub>sl</sub></i>	COPC loss constant due to leaching	See Equation C-5 (yr <sup>-1</sup> )
<i>k<sub>sv</sub></i>	COPC loss constant due to volatilization	0 yr <sup>-1</sup>

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### EQUATION C-3

#### SOIL LOSS CONSTANT DUE TO SOIL EROSION (SOIL INGESTION EQUATIONS)

$$kse = \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \left( \frac{Kd_s \cdot BD}{\Theta_{sw} + (Kd_s \cdot BD)} \right)$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$kse$	COPC loss constant due to soil erosion	0 yr <sup>-1</sup>
$0.1$	Units conversion factor	0.1 g·kg/cm <sup>2</sup> ·m <sup>2</sup>
$X_e$	Unit soil loss	See Equation C-17 (kg/m <sup>2</sup> ·yr)
$SD$	Sediment delivery ratio	Calculated using Equation C-18 (unitless)
$ER$	Soil enrichment ratio	Inorganics = 1 (unitless) Organics = 3 (unitless)
$BD$	Soil bulk density	1.5 g soil/cm <sup>3</sup> soil
$Z_s$	Soil mixing zone depth	Untilled = 1 cm
$Kd_s$	Soil-water partition coefficient	See Appendix B (mL [or cm <sup>3</sup> ] water/g soil)
$\Theta_{sw}$	Soil volumetric water content	0.2 mL water/cm <sup>3</sup> soil

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#### EQUATION C-4

#### COPC LOSS CONSTANT DUE TO RUNOFF (SOIL INGESTION EQUATIONS)

$$ksr = \frac{RO}{\Theta_{sw} \cdot Z_s} \cdot \left( \frac{1}{1 + \left( Kd_s \cdot \frac{BD}{\Theta_{sw}} \right)} \right)$$

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
<i>ksr</i>	COPC loss constant due to runoff	(yr <sup>-1</sup> )
<i>RO</i>	Average annual surface runoff from pervious areas	Site-specific (cm/yr)
<i>Θ<sub>sw</sub></i>	Soil volumetric water content	0.2 mL water/cm <sup>3</sup> soil
<i>Z<sub>s</sub></i>	Soil mixing zone depth	Untilled = 1 cm
<i>Kd<sub>s</sub></i>	Soil-water partition coefficient	See Appendix B (mL [or cm <sup>3</sup> ] water/g soil)
<i>BD</i>	Soil bulk density	1.5 g soil/cm <sup>3</sup> soil

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## EQUATION C-5

### SOIL LOSS CONSTANT DUE TO LEACHING (SOIL INGESTION EQUATIONS)

$$ksr = \frac{P + I - RO - E_v}{\Theta_{sw} \cdot Z_s \cdot \left[ 1.0 + \left( \frac{BD \cdot K_{ds}}{\Theta_{sw}} \right) \right]}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$ksl$	COPC loss constant due to leaching	(yr <sup>-1</sup> )
$P$	Average annual precipitation	18.06 to 164.19 cm/yr (Site-specific)
$I$	Average annual irrigation	0 to 100 cm/yr (Site-specific)
$RO$	Average annual surface runoff from pervious areas	Site-specific (cm/yr)
$E_v$	Average annual evapotranspiration	35 to 100 cm/yr (Site-specific)
$\Theta_{sw}$	Soil volumetric water content	0.2 mL water/cm <sup>3</sup> soil
$Z_s$	Soil mixing zone depth	Untilled = 1 cm
$K_{ds}$	Soil-water partition coefficient	See Appendix B (cm <sup>3</sup> water/g soil)
$BD$	Soil bulk density	1.5 g soil/cm <sup>3</sup> soil

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## EQUATION C-6

### COPC SOIL LOSS CONSTANT DUE TO VOLATILIZATION (SOIL INGESTION EQUATIONS)

$$k_{sv} = \left[ \frac{3.1536 \times 10^7 \cdot H}{Z_s \cdot KD_s \cdot R \cdot T_a \cdot BD} \right] \cdot \left[ 0.482 \cdot W^{0.78} \cdot \left( \frac{\mu_a}{\rho_a \cdot D_a} \right)^{-0.67} \cdot \left( \sqrt{\frac{4A}{\pi}} \right)^{-0.11} \right]$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$k_{sv}$	COPC soil constant due to volatilization	0 yr <sup>-1</sup>
0.482	Empirical constant	0.482 (unitless)
0.78	Empirical constant	0.78 (unitless)
-0.67	Empirical constant	-0.67 (unitless)
-0.11	Empirical constant	-0.11 (unitless)
$3.1536 \times 10^7$	Units conversion factor	$3.1536 \times 10^7$ s/yr
$H$	Henry's Law constant	See Appendix B (atm·m <sup>3</sup> /mol)
$Z_s$	Soil mixing zone depth	Untilled = 1 cm
$Kd_s$	Soil-water partition coefficient	See Appendix B (cm <sup>3</sup> water/g soil)
$R$	Universal gas constant	$8.205 \times 10^{-5}$ atm·m <sup>3</sup> /mol·K
$T_a$	Ambient air temperature	298 K
$BD$	Soil bulk density	1.5 g soil/cm <sup>3</sup> soil
$W$	Average annual wind speed	3.9 m/s

**EQUATION C-6 (Continued)**

**COPC SOIL LOSS CONSTANT DUE TO VOLATILIZATION  
(SOIL INGESTION EQUATIONS)**

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
$\mu_a$	Viscosity of air	$1.81 \times 10^{-4}$ g/cm-s
$\rho_a$	Density of air	0.0012 g/cm <sup>3</sup>
$D_a$	Diffusivity of COPC in air	See Appendix B (cm <sup>2</sup> /s)
$A$	Surface area of contaminated area	1.0 m <sup>2</sup>

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## EQUATION C-7

### DISSOLVED WATER PHASE CONCENTRATION (SURFACE WATER AND SEDIMENT EQUATIONS)

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$C_{dw}$	Dissolved water phase concentration	(mg COPC/L water)
$C_{wctot}$	Total COPC concentration in water column	Calculated using Equation C-8 (mg COPC/L water column)
$Kd_{sw}$	Suspended sediments/surface water partition coefficient	See Appendix B (L water/kg suspended sediment)
$TSS$	Total suspended solids concentration	2 to 300 mg/L (Site-specific)
$1 \times 10^{-6}$	Units conversion factor	$1 \times 10^{-6}$ kg/mg

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## EQUATION C-8

### TOTAL WATER COLUMN CONCENTRATION (SURFACE WATER AND SEDIMENT EQUATIONS)

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$C_{wctot}$	Total COPC concentration in water column	(mg COPC/L water column)
$f_{wc}$	Fraction of total water body COPC concentration in the water column	Calculated using Equation C-10 (unitless)
$C_{wtot}$	Total water body COPC concentration	Calculated using Equation C-25 (mg COPC/L water body [or g COPC/m <sup>3</sup> water body])
$d_{wc}$	Depth of water column	Site-specific (m)
$d_{bs}$	Depth of upper benthic sediment layer	0.03 m

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**EQUATION C-9**

**TOTAL WATER BODY LOAD**  
**(SURFACE WATER AND SEDIMENT EQUATIONS)**

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E$$

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
$L_T$	Total COPC load to the water body	(g/yr)
$L_{DEP}$	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body	Calculated using Equation C-12 (g/yr)
$L_{dif}$	Vapor phase COPC diffusion (dry deposition) load to water body	Calculated using Equation C-13 (g/yr)
$L_{RI}$	Runoff load from impervious surfaces	Calculated using Equation C-14 (g/yr)
$L_R$	Runoff load from pervious surfaces	Calculated using Equation C-15 (g/yr)
$L_E$	Soil erosion load	Calculated using Equation C-16 (g/yr)

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## EQUATION C-10

### FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) + d_{wc} / d_z + (\Theta_{bs} + Kd_{bs} \cdot C_{BS}) \cdot d_{bs} / d_z}$$

$$f_{bs} = 1 - f_{wc}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$f_{wc}$	Fraction of total water body COPC concentration in the water column	(unitless)
$f_{bs}$	Fraction of total water body COPC concentration in benthic sediment	(unitless)
$Kd_{sw}$	Suspended sediment/surface water partition coefficient	See Appendix B (L [or cm <sup>3</sup> ] water/kg suspended sediment)
$TSS$	Total suspended solids concentrations	2 to 300 mg/L (Site-specific)
$1 \times 10^{-6}$	Units conversion factor	$1 \times 10^{-6}$ kg/mg
$d_{wc}$	Depth of water column	Site-specific (m)
$d_{bs}$	Depth of upper benthic sediment layer	0.03 m
$d_z$	Total water body depth	Site-specific (m)
$C_{BS}$	Bed sediment concentration (or bed sediment bulk density)	1.0 g/cm <sup>3</sup> (or kg/L)
$\Theta_{bs}$	Bed sediment porosity	0.6 L <sub>water</sub> /L <sub>sediment</sub>

**EQUATION C-10 (Continued)**

**FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT  
(SURFACE WATER AND SEDIMENT EQUATIONS)**

$Kd_{bs}$

Bed sediment/sediment pore water partition coefficient

See Appendix B (L [or cm<sup>3</sup>] water/kg  
bottom sediment)

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### EQUATION C-11

#### OVERALL TOTAL WATER BODY DISSIPATION RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$k_{wt}$	Overall total water body dissipation rate constant	(yr <sup>-1</sup> )
$f_{wc}$	Total water column concentration	Calculated using Equation C-8 (unitless)
$k_v$	Water column volatilization rate constant	Calculated using Equation C-19 (yr <sup>-1</sup> )
$f_{bs}$	Fraction in water column and benthic sediment	Calculated using Equation C-10 (unitless)
$k_b$	Benthic burial rate constant	Calculated using Equation C-20 (yr <sup>-1</sup> )

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## EQUATION C-12

### DEPOSITION TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

$$L_{DEP} = Q \cdot [F_v \cdot Dy_{www} + (1.0 - F_v) \cdot Dy_{twp}] \cdot A_w$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$L_{DEP}$	Total (wet and dry) particle phase and wet vapor phase direct deposition load to water body	(g/yr)
$Q$	COPC specific emission rate	See Appendix A (g/s)
$F_v$	Fraction of COPC air concentration in vapor phase	See Appendix B (unitless)
$Dy_{www}$	Unitized yearly (water body or watershed) average wet deposition from particle phase	(s/m <sup>2</sup> -yr)
$Dy_{twp}$	Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase	(s/m <sup>2</sup> -yr)
$A_w$	Water body surface area	(m <sup>2</sup> )

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### EQUATION C-13

#### DIFFUSION LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cy_{wv} \cdot A_w \cdot 1 \times 10^{-6}}{\frac{H}{R \cdot T_{wk}}}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$L_{dif}$	Dry vapor phase diffusion load to water body	(g/yr)
$K_v$	Overall COPC transfer rate coefficient	Calculated using Equation C-21 (m/yr)
$Q$	COPC specific emission rate	See Appendix A (g/s)
$F_v$	Fraction of COPC air concentration in vapor phase	See Appendix B (unitless)
$Cy_{wv}$	Unitized yearly watershed air concentration from vapor phase	( $\mu\text{g-s/g-m}^3$ )
$A_w$	Water body surface area	Site-specific ( $\text{m}^2$ )
$10^{-6}$	Units conversion factor	$10^{-6} \text{ g}/\mu\text{g}$
$H$	Henry's Law constant	See Appendix B ( $\text{atm-m}^3/\text{mol}$ )
$R$	Universal gas constant	$8.205 \times 10^{-5} \text{ atm-m}^3/\text{mol-K}$
$T_{wk}$	Water body temperature	298 K

# EQUATION C-14

## IMPERVIOUS RUNOFF LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

$$L_{RI} = Q \cdot [F_v \cdot Dy_{www} + (1.0 - F_v) \cdot Dy_{twp}] \cdot A_I$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$L_{RI}$	Runoff load from impervious surfaces	(g/yr)
$Q$	COPC specific emission rate	See Appendix A (g/s)
$F_v$	Fraction of COPC air concentration in vapor phase	See Appendix B (unitless)
$Dy_{www}$	Unitized yearly (water body or watershed) average wet deposition from vapor phase	(s/m <sup>2</sup> -yr)
$Dy_{twp}$	Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase	(s/m <sup>2</sup> -yr)
$A_I$	Impervious watershed area receiving COPC deposition	Site-specific (m <sup>2</sup> )

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## EQUATION C-15

### PERVIOUS RUNOFF LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\Theta_{sw} + Kd_s \cdot BD} \cdot 0.01$$

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
$L_R$	Runoff load from pervious surfaces	(g/yr)
$RO$	Average annual surface runoff from pervious areas	Site-specific (cm/yr)
$A_L$	Total watershed area receiving COPC deposition	Site-specific (m <sup>2</sup> )
$A_I$	Impervious watershed area receiving COPC deposition	Site-specific (m <sup>2</sup> )
$Cs$	Average soil concentration over exposure duration	Calculated using Equation C-1 (mg COPC/kg soil)
$BD$	Soil bulk density	1.5 g soil/cm <sup>3</sup> soil
$\Theta_{sw}$	Soil volumetric water content	0.2 mL water/cm <sup>3</sup> soil
$Kd_s$	Soil-water partition coefficient	See Appendix B (cm <sup>3</sup> water/g soil)
$0.01$	Units conversion factor	0.01 kg-cm <sup>2</sup> /mg-m <sup>2</sup>

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## EQUATION C-16

### EROSION LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\Theta_{sw} + Kd_s \cdot BD} \cdot 0.001$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$L_E$	Soil erosion load	(g/yr)
$X_e$	Unit soil loss	Calculated using Equation C-17 (kg/m <sup>2</sup> -yr)
$A_L$	Total watershed area receiving deposition	Site-specific (m <sup>2</sup> )
$A_I$	Area of impervious watershed receiving deposition	Site-specific (m <sup>2</sup> )
$SD$	Watershed sediment delivery ratio	Calculated using Equation C-18 (unitless)
$ER$	Soil enrichment ratio	Inorganic COPCs = 1 (unitless) Organic COPCs = 3 (unitless)
$Cs$	Average soil concentration over exposure duration	Calculated using Equation C-1 (mg COPC/kg soil)
$Kd_s$	Soil-water partition coefficient	See Appendix B (mL [or cm <sup>3</sup> ] water/g soil)
$BD$	Soil bulk density	1.5 g/cm <sup>3</sup>
$\Theta_{sw}$	Soil volumetric water content	0.2 mL water/cm <sup>3</sup> soil
0.001	Units conversion factor	0.001 kg-cm <sup>2</sup> /mg-m <sup>3</sup>

# EQUATION C-17

## UNIVERSAL SOIL LOSS EQUATION (USLE) (SURFACE WATER AND SEDIMENT EQUATIONS)

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$X_e$	Unit soil loss	(kg/m <sup>2</sup> -yr)
$RF$	USLE rainfall (or erosivity) factor	50 to 300 yr <sup>-1</sup> (Site-specific)
$K$	USLE erodibility factor	Site-specific (ton/acre)
$LS$	USLE length-slope factor	Site-specific (unitless)
$C$	USLE cover management factor	Site-specific (unitless)
$PF$	USLE supporting practice factor	Site-specific (unitless)
907.18	Units conversion factor	907.18 kg/ton
4047	Units conversion factor	4047 m <sup>2</sup> /acre

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# EQUATION C-18

## SEDIMENT DELIVERY RATIO (SURFACE WATER AND SEDIMENT EQUATIONS)

$$SD = a \cdot (A_L)^{-b}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
<i>SD</i>	Watershed sediment delivery ratio	(unitless)
<i>a</i>	Empirical intercept coefficient	Watershed Area (mi <sup>2</sup> ) “ <i>a</i> ” Coefficient (unitless) ≤ 0.1 2.1 > 0.1 but ≤ 1.0 1.9 > 1.0 but ≤ 10 1.4 > 10 but ≤ 100 1.2 > 100 0.6
<i>A<sub>L</sub></i>	Total watershed area receiving deposition	Site-specific (m <sup>2</sup> )
<i>b</i>	Empirical slope coefficient	0.125 (unitless)

### EQUATION C-19

#### WATER COLUMN VOLATILIZATION LOSS RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$k_v$	Water column volatilization rate constant	(yr <sup>-1</sup> )
$K_v$	Overall COPC transfer rate coefficient	Calculated using Equation C-21 (m/yr)
$Kd_{sw}$	Suspended sediment/surface water partition coefficient	See Appendix B (L water/kg suspended sediments)
$d_z$	Total water body depth	Site-specific (m)
$TSS$	Total suspended solids concentration	2 to 300 mg/L (Site-specific)
$1 \times 10^{-6}$	Units conversion factor	$1 \times 10^{-6}$ kg/mg

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## EQUATION C-20

### BENTHIC BURIAL RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

$$k_b = \left( \frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_w \cdot TSS} \right) \cdot \left( \frac{TSS \cdot 1 \times 10^{-6}}{C_{BS} \cdot d_{bs}} \right)$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$k_b$	Benthic burial rate constant	(yr <sup>-1</sup> )
$X_e$	Unit soil loss	Calculated using Equation C-17 (kg/m <sup>2</sup> -yr)
$A_L$	Total watershed area receiving deposition	Site-specific (m <sup>2</sup> )
$SD$	Watershed sediment delivery ratio	Calculated using Equation C-18 (unitless)
$1 \times 10^3$	Units conversion factor	1 × 10 <sup>3</sup> g/kg
$Vf_x$	Average volumetric flow rate through water body	Site-specific (m <sup>3</sup> /yr)
$TSS$	Total suspended solids concentration	2 to 300 mg/L (Site-specific)
$A_w$	Water body surface area	Site-specific (m <sup>2</sup> )
$1 \times 10^{-6}$	Units conversion factor	1 × 10 <sup>-6</sup> kg/mg
$C_{BS}$	Bed sediment concentration	1.0 g/cm <sup>3</sup>
$d_{bs}$	Depth of upper benthic sediment layer	0.03 m

## EQUATION C-21

### OVERALL COPC TRANSFER RATE COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

$$K_v = \left[ K_L^{-1} + \left( K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right]^{-1} \cdot \Theta^{(T_{wk} - 293)}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$K_v$	Overall COPC transfer rate coefficient	(m/yr)
$K_L$	Liquid phase transfer coefficient	Calculated using Equation C-22 (m/yr)
$K_G$	Gas phase transfer coefficient	Calculated using Equation C-23 (m/yr)
$H$	Henry's Law constant	See Appendix B (atm-m <sup>3</sup> /mol)
$R$	Universal gas constant	8.205x10 <sup>-5</sup> atm-m <sup>3</sup> /mol-K
$T_{wk}$	Water body temperature	298 K
$\Theta$	Temperature correction factor	1.026 (unitless)

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## EQUATION C-22

### LIQUID PHASE TRANSFER COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

**For flowing streams or rivers**

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7$$

**For quiescent lakes or ponds**

$$K_L = (C_d^{0.5} \cdot W) \cdot \left( \frac{\rho_a}{\rho_w} \right)^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left( \frac{\mu_w}{\rho_w \cdot D_w} \right)^{-0.67} \cdot 3.1536 \times 10^7$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$K_L$	Liquid phase transfer coefficient	(m/yr)
$D_w$	Diffusivity of COPC in water	See Appendix B (cm <sup>2</sup> /s)
$U$	Current velocity	Site-specific (m/s)
$d_z$	Total water body depth	Site-specific (m)
$3.1536 \times 10^7$	Units conversion factor	$3.1536 \times 10^7$ s/yr
$C_d$	Drag coefficient	0.0011 (unitless)
$W$	Average annual wind speed	3.9 m/s

**EQUATION C-22 (Continued)**

**LIQUID PHASE TRANSFER COEFFICIENT  
(SURFACE WATER AND SEDIMENT EQUATIONS)**

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
$\rho_a$	Density of air	0.0012 g/cm <sup>3</sup>
$\rho_w$	Density of water	1 g/cm <sup>3</sup>
$k$	von Karman's constant	0.4 (unitless)
$\lambda_z$	Dimensionless viscous sublayer thickness	4 (unitless)
$\mu_w$	Viscosity of water corresponding to water temperature	1.69x10 <sup>-2</sup> g/cm-s

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## EQUATION C-23

### GAS PHASE TRANSFER COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

**For flowing streams and rivers**

$$K_G = 36500 \text{ m / yr}$$

**For quiescent lakes or ponds**

$$K_G = \left( C_d^{0.5} \cdot W \right) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left( \frac{\mu_a}{\rho_a \cdot D_a} \right)^{-0.67} \cdot 3.1536 \times 10^7$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$K_G$	Gas phase transfer coefficient	(m/yr)
$C_d$	Drag coefficient	0.0011 (unitless)
$W$	Average annual wind velocity	3.9 m/s
$k$	von Karman's constant	0.4 (unitless)
$\lambda_z$	Dimensionless viscous sublayer thickness	4 (unitless)
$\mu_a$	Viscosity of air	$1.81 \times 10^{-4}$ g/cm-s
$\rho_a$	Density of air	$0.0012 \text{ g/cm}^3$
$D_a$	Diffusivity of COPC in air	See Appendix B ( $\text{cm}^2/\text{s}$ )
$3.1536 \times 10^7$	Units conversion factor	$3.1536 \times 10^7 \text{ s/yr}$

## EQUATION C-24

### COPC CONCENTRATION IN BED SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

$$C_{sb} = f_{bs} \cdot C_{wtot} \cdot \frac{Kd_{bs}}{\Theta_{bs} + Kd_{bs} \cdot C_{BS}} \cdot \frac{d_{wc} + d_{bs}}{d_{bs}}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
$C_{sb}$	Concentration sorbed to bed sediment	(mg COPC/kg sediment)
$f_{bs}$	Fraction benthic sediment in water column and bed sediment	Calculated using Equation C-10 (unitless)
$C_{wtot}$	Total water body concentration	Calculated using Equation C-25 (mg COPC/ L water body [or g COPC/cm <sup>3</sup> water body])
$Kd_{bs}$	Bed sediment/sediment pore water partition coefficient	See Appendix B (L water/kg bed sediment [or cm <sup>3</sup> water/g bed sediment])
$\Theta_{bs}$	Bed sediment porosity	0.6 (unitless [L <sub>pore volume</sub> /L <sub>sediment</sub> ])
$C_{BS}$	Bed sediment concentration (or sediment bulk density)	1.0 g/cm <sup>3</sup>
$d_{wc}$	Depth of water column	Site-specific (m)
$d_{bs}$	Depth of upper benthic sediment layer	0.03 m

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## EQUATION C-25

### TOTAL WATER BODY CONCENTRATION (SURFACE WATER AND SEDIMENT EQUATIONS)

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} \cdot k_{wt} \cdot A_w \cdot (d_{wc} + d_{bs})}$$

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
$C_{wtot}$	Total water body COPC concentration, including water column and bed sediment	(g COPC/m <sup>3</sup> water body [equivalent to mg COPC/L water body])
$L_T$	Total COPC load to the water body, including deposition, runoff, and erosion	Calculated using Equation C-9 (g/yr)
$Vf_x$	Average volumetric flow rate through water body	Site-specific (m <sup>3</sup> /yr)
$f_{wc}$	Fraction of water body COPC concentration in the water column	0 to 1(unitless); Calculated using Equation C-10
$k_{wt}$	Overall total water body dissipation rate constant	Calculated using Equation C-11 (yr <sup>-1</sup> )
$A_w$	Water body surface area	Site-specific (m <sup>2</sup> )
$d_{wc}$	Depth of water column	Site-specific (m)
$d_{bs}$	Depth of upper benthic sediment layer	0.03 m

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## EQUATION C-26

### PLANT CONCENTRATION DUE TO DIRECT DEPOSITION (TERRESTRIAL PLANT EQUATIONS)

$$Pd = \frac{1000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)]}{Yp \cdot kp}$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
<i>Pd</i>	Concentration of COPC in plant due to direct (wet and dry) deposition	(mg COPC)
<i>1000</i>	Units conversion factor	1000 mg/g
<i>Q</i>	COPC specific emission rate	See Appendix A (g/s)
<i>F<sub>v</sub></i>	Fraction of COPC air concentration in vapor phase	See Appendix B (unitless)
<i>Dydp</i>	Unitized yearly average dry deposition from particle phase	(s/m <sup>2</sup> -yr)
<i>Rp</i>	Interception fraction of the edible portion of the plant	0.39 (unitless)
<i>Fw</i>	Fraction of COPC wet deposition that adheres to plant surfaces	Anions = 0.2 (unitless) Cations and most Organics = 0.6 (unitless)
<i>Dywp</i>	Unitized yearly wet deposition in particle phase	(s/m <sup>2</sup> -yr)
<i>kp</i>	Plant surface loss coefficient	18 yr <sup>-1</sup>
<i>Tp</i>	Length of plant exposure to deposition per harvest of edible plant portion	0.164 yr
<i>Yp</i>	Yield or standing crop biomass of the edible portion of the plant (productivity)	2.24 kg DW/m <sup>2</sup>

# **EQUATION C-27**

## **PLANT CONCENTRATION DUE TO AIR-TO-PLANT TRANSFER (TERRESTRIAL PLANT EQUATIONS)**

$$P_v = Q \cdot F_v \cdot \frac{C_{yv} \cdot B_v \cdot VG}{\rho_a}$$

<b><u>Variable</u></b>	<b><u>Description</u></b>	<b><u>Value and Units</u></b>
$P_v$	Concentration of COPC in plant due to air-to-plant transfer	µg COPC/g DW (equivalent to mg COPC/kg DW)
$Q$	COPC-specific emission rate	See Appendix A (g/s)
$F_v$	Fraction of COPC air concentration in vapor phase	See Appendix B (unitless)
$C_{yv}$	Unitized yearly average air concentration from vapor phase	(µg-s/g-m <sup>3</sup> )
$B_v$	COPC air-to-plant biotransfer factor	See Appendix B (unitless) or (mg COPC/g DW)/ (mg COPC/g DW)
$VG$	Empirical correction factor	COPCs with a log K <sub>ow</sub> > 4 = 0.01 (unitless) COPCs with a log K <sub>ow</sub> < 4 = 1.0 (unitless)
$\rho_a$	Density of air	1200.0 g/m <sup>3</sup>

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### EQUATION C-28

#### PLANT CONCENTRATION DUE TO ROOT UPTAKE (TERRESTRIAL PLANT EQUATIONS)

$$Pr = Cs \cdot Br$$

<u>Variable</u>	<u>Description</u>	<u>Value and Units</u>
<i>Pr</i>	Concentration of COPC in plant due to root uptake	(mg COPC/kg DW)
<i>Cs</i>	Average soil concentration over exposure duration	Calculated using Equation C-1 (mg COPC/kg soil)
<i>Br</i>	Plant-soil bioconcentration factor	See Appendix B (unitless or [mg COPC/kg DW plant]/[mg COPC/kg soil])

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